Ali Alavi

List of Publications by Year
in descending order

88 papers	5,859 citations	76294 40 h-index	74108 75 g-index
90 all docs	90 docs citations	90 times ranked	3361 citing authors

#	Article	IF	Citations
1	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
2	Fermion Monte Carlo without fixed nodes: A game of life, death, and annihilation in Slater determinant space. Journal of Chemical Physics, 2009, 131, 054106.	1.2	567
3	Towards an exact description of electronic wavefunctions in real solids. Nature, 2013, 493, 365-370.	13.7	440
4	Communications: Survival of the fittest: Accelerating convergence in full configuration-interaction quantum Monte Carlo. Journal of Chemical Physics, 2010, 132, 041103.	1.2	308
5	Semistochastic Heat-Bath Configuration Interaction Method: Selected Configuration Interaction with Semistochastic Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 1595-1604.	2.3	232
6	Ab InitioMolecular Dynamics with Excited Electrons. Physical Review Letters, 1994, 73, 2599-2602.	2.9	227
7	Combining the Complete Active Space Self-Consistent Field Method and the Full Configuration Interaction Quantum Monte Carlo within a Super-CI Framework, with Application to Challenging Metal-Porphyrins. Journal of Chemical Theory and Computation, 2016, 12, 1245-1258.	2.3	156
8	Breaking the carbon dimer: The challenges of multiple bond dissociation with full configuration interaction quantum Monte Carlo methods. Journal of Chemical Physics, 2011, 135, 084104.	1.2	134
9	Reconstruction of charged surfaces: General trends and a case study of Pt(110) and Au(110). Physical Review B, 2003, 68, .	1.1	125
10	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. Journal of Chemical Theory and Computation, 2011, 7, 2780-2785.	2.3	117
11	Approaching chemical accuracy using full configuration-interaction quantum Monte Carlo: A study of ionization potentials. Journal of Chemical Physics, 2010, 132, 174104.	1.2	110
12	Convergence of many-body wave-function expansions using a plane-wave basis: From homogeneous electron gas to solid state systems. Physical Review B, 2012, 86, .	1.1	101
13	Full configuration interaction perspective on the homogeneous electron gas. Physical Review B, 2012, 85, .	1.1	99
14	Linear-scaling and parallelisable algorithms for stochastic quantum chemistry. Molecular Physics, 2014, 112, 1855-1869.	0.8	92
15	Unbiased reduced density matrices and electronic properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2014, 141, 244117.	1.2	90
16	The Ground State Electronic Energy of Benzene. Journal of Physical Chemistry Letters, 2020, 11, 8922-8929.	2.1	90
17	A study of electron affinities using the initiator approach to full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2011, 134, 024112.	1.2	89
18	Investigation of the full configuration interaction quantum Monte Carlo method using homogeneous electron gas models. Journal of Chemical Physics, 2012, 136, 244101.	1.2	86

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19	Stochastic Multiconfigurational Self-Consistent Field Theory. Journal of Chemical Theory and Computation, 2015, 11, 5316-5325.	2.3	86
20	Semi-stochastic full configuration interaction quantum Monte Carlo: Developments and application. Journal of Chemical Physics, 2015, 142, 184107.	1.2	83
21	Taming the First-Row Diatomics: A Full Configuration Interaction Quantum Monte Carlo Study. Journal of Chemical Theory and Computation, 2012, 8, 4138-4152.	2.3	77
22	An excited-state approach within full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 134117.	1.2	77
23	Understanding the Mechanism Stabilizing Intermediate Spin States in Fe(II)-Porphyrin. Journal of Physical Chemistry A, 2018, 122, 4935-4947.	1.1	75
24	Where do the H atoms reside in PdHxsystems?. Molecular Physics, 2003, 101, 1781-1787.	0.8	71
25	Multireference linearized coupled cluster theory for strongly correlated systems using matrix product states. Journal of Chemical Physics, 2015, 143, 102815.	1.2	67
26	Explicitly correlated plane waves: Accelerating convergence in periodic wavefunction expansions. Journal of Chemical Physics, 2013, 139, 084112.	1.2	62
27	Full Configuration Interaction Excitations of Ethene and Butadiene: Resolution of an Ancient Question. Journal of Chemical Theory and Computation, 2012, 8, 4441-4451.	2.3	57
28	Unbiasing the initiator approximation in full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2019, 151, 224108.	1.2	56
29	Combining Internally Contracted States and Matrix Product States To Perform Multireference Perturbation Theory. Journal of Chemical Theory and Computation, 2017, 13, 488-498.	2.3	55
30	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. Journal of Chemical Physics, 2020, 153, 034107.	1.2	55
31	Krylov-Projected Quantum MonteÂCarlo Method. Physical Review Letters, 2015, 115, 050603.	2.9	53
32	Combining the Transcorrelated Method with Full Configuration Interaction Quantum Monte Carlo: Application to the Homogeneous Electron Gas. Journal of Chemical Theory and Computation, 2018, 14, 1403-1411.	2.3	52
33	Mechanism for the high reactivity of CO oxidation on a rutheniumâ€“oxide. Journal of Chemical Physics, 2001, 114, 5956-5957.	1.2	51
34	Role of Valence and Semicore Electron Correlation on Spin Gaps in Fe(II)-Porphyrins. Journal of Chemical Theory and Computation, 2019, 15, 1492-1497.	2.3	51
35	An explicitly correlated approach to basis set incompleteness in full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2012, 137, 164112.	1.2	49
36	Efficient formulation of full configuration interaction quantum Monte Carlo in a spin eigenbasis via the graphical unitary group approach. Journal of Chemical Physics, 2019, 151, 094104.	1.2	49

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37	Density matrices in full configuration interaction quantum Monte Carlo: Excited states, transition dipole moments, and parallel distribution. Journal of Chemical Physics, 2017, 146, 244105.	1.2	47
38	Charge-transfer molecular dynamics. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1992, 65, 489-500.	0.6	45
39	Compact numerical solutions to the two-dimensional repulsive Hubbard model obtained via nonunitary similarity transformations. Physical Review B, 2019, 99, .	1.1	43
40	AccurateAbÂInitioCalculation of Ionization Potentials of the First-Row Transition Metals with the Configuration-Interaction Quantum MonteÂCarlo Technique. Physical Review Letters, 2015, 114, 033001.	2.9	42
41	Similarity transformation of the electronic SchrÃ¶dinger equation via Jastrow factorization. Journal of Chemical Physics, 2019, 151, 061101.	1.2	40
42	Two interacting electrons in a box: An exact diagonalization study. Journal of Chemical Physics, 2000, 113, 7735-7745.	1.2	39
43	Electronic correlations and magnetic interactions in infinite-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NdNiO</mml:mi><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2020, 102, .	1.1	38
44	Two interacting electrons in a spherical box:â€, An exact diagonalization study. Physical Review B, 2002, 66, .	1.1	36
45	Stochastic multi-reference perturbation theory with application to the linearized coupled cluster method. Journal of Chemical Physics, 2017, 146, 044107.	1.2	35
46	The adaptive shift method in full configuration interaction quantum Monte Carlo: Development and applications. Journal of Chemical Physics, 2020, 153, 224115.	1.2	33
47	The Intricate Case of Tetramethyleneethane: A Full Configuration Interaction Quantum Monte Carlo Benchmark and Multireference Coupled Cluster Studies. Journal of Chemical Theory and Computation, 2018, 14, 2439-2445.	2.3	28
48	Compression of Spin-Adapted Multiconfigurational Wave Functions in Exchange-Coupled Polynuclear Spin Systems. Journal of Chemical Theory and Computation, 2020, 16, 2202-2215.	2.3	28
49	Molecular-dynamics simulation of methane adsorbed on MgO: Evidence for a Kosterlitz-Thouless transition. Molecular Physics, 1990, 71, 1173-1191.	0.8	27
50	Projector Quantum MonteÂCarlo Method for Nonlinear Wave Functions. Physical Review Letters, 2017, 118, 176403.	2.9	25
51	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Ironâ€“Sulfur Clusters. Journal of Chemical Theory and Computation, 2021, 17, 5684-5703.	2.3	25
52	Entropy of H2O Wetting Layersâ€. Journal of Physical Chemistry B, 2004, 108, 14362-14367.	1.2	24
53	Analytic nuclear forces and molecular properties from full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 143, 054108.	1.2	24
54	FCIQMC-Tailored Distinguishable Cluster Approach. Journal of Chemical Theory and Computation, 2020, 16, 5621-5634.	2.3	22

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55	Resolution of Low-Energy States in Spin-Exchange Transition-Metal Clusters: Case Study of Singlet States in [Fe(III)₄S₄] Cubanes. Journal of Physical Chemistry A, 2021, 125, 4727-4740.	1.1	22
56	Chemical insights into the electronic structure of Fe(<scp>II</scp>) porphyrin using <scp>FCIQMC</scp>, <scp>DMRG</scp>, and generalized active spaces. International Journal of Quantum Chemistry, 2021, 121, e26454.	1.0	21
57	Assessment of multireference approaches to explicitly correlated full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2016, 145, 054117.	1.2	20
58	Correlation energies of the high-density spin-polarized electron gas to meV accuracy. Physical Review B, 2018, 98, .	1.1	20
59	Molecular-dynamics simulation of argon physisorbed on magnesium oxide. Molecular Physics, 1990, 69, 703-713.	0.8	18
60	Accelerating the convergence of exact diagonalization with the transcorrelated method: Quantum gas in one dimension with contact interactions. Physical Review A, 2018, 98, .	1.0	18
61	Binding curve of the beryllium dimer using similarity-transformed FCIQMC: Spectroscopic accuracy with triple-zeta basis sets. Journal of Chemical Physics, 2021, 155, 011102.	1.2	18
62	Transcorrelated coupled cluster methods. Journal of Chemical Physics, 2021, 155, 191101.	1.2	17
63	Nonlinear biases, stochastically sampled effective Hamiltonians, and spectral functions in quantum Monte Carlo methods. Physical Review B, 2018, 98, .	1.1	16
64	A comparative study using state-of-the-art electronic structure theories on solid hydrogen phases under high pressures. Npj Computational Materials, 2019, 5, .	3.5	16
65	Towards efficient and accurate ab initio solutions to periodic systems via transcorrelation and coupled cluster theory. Physical Review Research, 2021, 3, .	1.3	16
66	Small polarons and the Janus nature of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml (110). Physical Review B, 2020, 101, .	1.1	15
67	Eliminating the wave-function singularity for ultracold atoms by a similarity transformation. Physical Review Research, 2020, 2, .	1.3	15
68	Dynamics of quantum tunneling: Effects on the rate and transition path of OH on Cu(110). Physical Review B, 2010, 81, .	1.1	14
69	Insights into the structure of many-electron wave functions of Mott-insulating antiferromagnets: The three-band Hubbard model in full configuration interaction quantum Monte Carlo. Physical Review B, 2015, 91, .	1.1	14
70	Time Propagation and Spectroscopy of Fermionic Systems Using a Stochastic Technique. Physical Review Letters, 2018, 121, 056401.	2.9	14
71	The color center singlet state of oxygen vacancies in TiO2. Journal of Chemical Physics, 2020, 153, 204704.	1.2	13
72	Population control bias and importance sampling in full configuration interaction quantum Monte Carlo. Physical Review B, 2021, 103, .	1.1	11

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73	A full configuration interaction quantum Monte Carlo study of ScO, TiO, and VO molecules. Journal of Chemical Physics, 2021, 154, 164302.	1.2	11
74	Preface: Special Topic Section on Advanced Electronic Structure Methods for Solids and Surfaces. Journal of Chemical Physics, 2015, 143, 102601.	1.2	10
75	Enhancement of superexchange due to synergetic breathing and hopping in corner-sharing cuprates. Nature Physics, 2022, 18, 190-195.	6.5	10
76	General embedded cluster protocol for accurate modeling of oxygen vacancies in metal-oxides. Journal of Chemical Physics, 2022, 156, 124704.	1.2	9
77	Combined unitary and symmetric group approach applied to low-dimensional Heisenberg spin systems. Physical Review B, 2022, 105, .	1.1	9
78	Full configuration interaction quantum Monte Carlo treatment of fragments embedded in a periodic mean field. Journal of Chemical Physics, 2022, 156, 154107.	1.2	8
79	Spin Purification in Full-CI Quantum Monte Carlo via a First-Order Penalty Approach. Journal of Physical Chemistry A, 2022, 126, 2050-2060.	1.1	8
80	Performance of a one-parameter correlation factor for transcorrelation: Study on a series of second row atomic and molecular systems. Journal of Chemical Physics, 2022, 156, .	1.2	8
81	Benchmark study of Nagaoka ferromagnetism by spin-adapted full configuration interaction quantum Monte Carlo. Physical Review B, 2021, 104, .	1.1	6
82	Ammonium cyanate: a DFT study of crystal structure, rotational barriers and vibrational spectrum. Molecular Physics, 2004, 102, 869-876.	0.8	5
83	Signatures of the BCS-BEC crossover in the yrast spectra of Fermi quantum rings. Physical Review Research, 2021, 3, .	1.3	5
84	Synthesis and extensive characterisation of phosphorus doped graphite. RSC Advances, 2016, 6, 62140-62145.	1.7	4
85	FCIQMC-Tailored Distinguishable Cluster Approach: Open-Shell Systems. Journal of Chemical Theory and Computation, 2022, , .	2.3	4
86	Are smooth pseudopotentials a good choice for representing short-range interactions?. Physical Review A, 2019, 99, .	1.0	3
87	The use of XANES and ELNES for the Characterisation of Stabilised Zirconia. Materials Research Society Symposia Proceedings, 2001, 699, 821.	0.1	1
88	Ab Initio Wavefunction Analysis of Electron Removal Quasi-Particle State of NdNiO2 With Fully Correlated Quantum Chemical Methods. Frontiers in Physics, 2022, 10, .	1.0	0